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LIAPUNOV STABILITY OF DISTRIBUTED
PARAMETER SYSTEMS

by



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A THESIS

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The undersigned certify that they have
read, and recommend to the Faculty of Graduate
Studies for acceptance, a thesis entitled Liapunov
Stability of Distributed Parameter Systems sub-
mitted by T. Wayne Lee in partial fulfilment of
the requirements for the degree of Master of
Science.

ABSTRACT

During the past few years, interest in studying stability of distributed parameter systems via Liapunov's second method has slowly been forming. In this thesis two techniques are developed for finding Liapunov functionals for certain types of distributed systems. In the first technique, the use of a non-identity matrix in a Liapunov functional of quadratic form proves to be more successful than methods used in which the weighting matrix was replaced by the identity matrix. The second technique is an extension to the variable gradient method of generating Liapunov functions. A systematic algorithm analogous to the one used for lumped systems is developed and illustrated by two examples.

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LIST OF MAJOR SYMBOLS

Symbol	Meaning
\underline{f}	vector function of system variables
H	integrand of Liapunov functional
\underline{I}	identity matrix
N	Lewis number
N_p	Peclet number
\underline{R}	state vector
s	normalized reactor distance variable
t	time
T	temperature
\underline{U}	perturbation state vector
u	concentration perturbation
v	temperature perturbation
\underline{X}	vector of spatial coordinates
x	element of \underline{X}
y	dimensionless concentration
z	dimensionless temperature

Greek Letters

α, ν	normalizing constants
β	heat of reaction coefficient
γ	reduced activation energy
η	reduced temperature variable
ξ	reduced concentration variable
ϕ^2	Thiele modulus
Ω	spatial domain

<u>Symbol</u>	<u>Meaning</u>
---------------	----------------

Subscripts

- | | |
|------|-----------------------|
| 0 | initial condition |
| e | equilibrium condition |

Superscripts

- | | |
|---|--------------------------------------|
| . | differentiation with respect to time |
| * | steady state condition |
| T | transpose |

CHAPTER 1

REVIEW OF STABILITY METHODS
FOR DISTRIBUTED PARAMETER SYSTEMS1.1 Need For Stability Analysis

A system is said to be a distributed parameter system if its variables depend both on time and the spatial coordinates. If the spatial dependence is sufficiently small that it can be neglected, then the system is called a lumped parameter system. For a distributed parameter system, usually the governing equations are partial differential equations, while, for a lumped system, these equations reduce to ordinary differential equations.

One of the difficulties in controlling physical systems is encountered in assuring adequate stability. A qualitative definition of stability is as follows

DEFINITION

A system with a suitable response to a set of inputs and initial conditions, is said to be stable if it returns to a new response, close to the original, whenever small changes occur in the inputs and/or initial conditions.

Currently, much of the work on stability of distributed parameter systems comes from the area of process control. The review papers of Aris^{1*} and Lapidus¹⁹ cover

*

Numbers placed above the line of text refer to the references. Only those works relevant to this thesis are listed. For an extensive bibliography on stability of distributed parameter systems see Wang³³.

the major works, many of which were published within the past five years. Systems in process control which are characterized by, say, diffusion or conduction are well suited to be analysed as distributed parameter systems.

The need for stability analysis of distributed parameter systems is also found in the areas of aerospace vehicles and continuous furnaces³², panel flutter in supersonic flow²⁷, vibrating shafts²⁸, and electrical power transmission lines^{6,32}. In processes where temperature and pressure, say, are variables it is obviously necessary to ensure that these variables are maintained within given bounds.

Aerospace re-entry vehicles use ablative shields to protect the space capsule from aerodynamic heating. This is an example of a variable-domain distributed parameter system in which the domain boundary motion depends upon certain system variables such as velocity, evaluated at the boundary. Continuous furnaces are used in drying and heat treating processes. It is necessary to maintain close control of the temperature distribution of a uniform material strip inside a furnace by means of varying the velocity of the transport mechanism. The electrical power transmission line is an example of a fixed domain distributed parameter system where it is required to closely regulate the load voltage and generator frequency.

1.2 Different Types Of Stability

Basically, there are two main types of stability which are covered in the literature; bounded input-bounded output, and null state or Liapunov stability. The former type has been investigated by several authors. Zames³⁸ used functional analysis methods to solve the output stability of certain nonlinear time-varying systems.

Others^{16,22-25} have used the maximum principle for parabolic equations²⁶ to extend the work of Bellman³ on the nonlinear equation of heat conduction. Kastenborg¹³⁻¹⁵ used the method of comparison theorems to solve the stability problem for a class of nonlinear feedback control systems governed by parabolic partial differential equations.

This type of stability will not be discussed further here. In this thesis only Liapunov stability will be investigated. Suffice it to say, however, that, as shown by De Figueiredo⁶, bounded input-bounded output stability can be deduced under certain conditions, from asymptotic stability. The basic concepts involved in Liapunov stability are discussed in the following section.

1.3 Liapunov Stability

a) Lumped systems

For a system of ordinary differential equations,

$$\dot{\underline{R}} = \underline{f}(\underline{R}) ,$$

the following is the so-called ϵ, δ definition of stability in the sense of Liapunov;

DEFINITION¹¹

An equilibrium state \underline{R}_e of a free dynamic system is stable if for every real number $\epsilon > 0$ there exists a real number $\delta(\epsilon, t_0) > 0$ such that

$$\|\underline{R}_0 - \underline{R}_e\| \leq \delta$$

implies

$$\|\underline{\phi}(t; \underline{R}_0, t_0) - \underline{R}_e\| \leq \epsilon \quad \text{for all } t \geq t_0$$

where \underline{R}_0 is the initial state vector, $\underline{\phi}$ is the solution vector of the above system of differential equations and $\|\cdot\|$ represents a norm or metric.

If, in addition to the above definition, the following holds:

$$\|\underline{\phi}(t; \underline{R}_0, t_0) - \underline{R}_e\| \rightarrow 0 \text{ as } t \rightarrow \infty$$

then the equilibrium state \underline{R}_e is said to be asymptotically stable.

The idea of the Liapunov technique is to mathematically describe a kind of distribution of stored energy of a system. It is the purpose of the direct method of Liapunov to determine whether this energy decreases toward a minimum value or toward zero. If this can be shown, the steady state of the system is stable or asymptotically stable, respectively. The steady state of a free dynamic system described by ordinary differential equations is defined by a point in the phase diagram of the state variables.

The method consists of choosing a scalar function

$V(\underline{R})$ (Liapunov function) of the state variables which has a definite sign. If the sign of the time derivative of this function is semi-definite or definite and of the opposite sign then the steady state of the system is stable or asymptotically stable, respectively. Thus, knowledge of the system stability is found without having to solve the transient equations.

The disadvantage of this technique is that it yields only a sufficient condition for stability. If the sign definiteness criteria are not met, nothing can be concluded about the stability of the system. When this happens, another function must be chosen as a Liapunov function and try the technique again.

For linear stationary systems it has been found that for global asymptotic stability, the following Liapunov function is both necessary and sufficient.

$$V(\underline{R}) = \underline{R}^T \underline{P} \underline{R}$$

where \underline{P} is a positive definite symmetric matrix.

Methods for determining stability of these constant linear systems are well established. Many excellent books covering the subject are available, including Hahn¹¹, Krasovskii¹⁷ and LaSalle and Lefschetz²⁰, to mention a few. Although general nonlinear systems cannot yet be treated satisfactorily, Liapunov stability theory has helped to identify various time-varying and nonlinear models with well-established qualitative

behavior. Brockett, in his survey paper⁵ discusses many of these models in detail. Many of the design techniques of classical control theory, such as, Nyquist's criterion, Root-Locus and Root-Contour methods¹⁸, all are directly or indirectly related to the circle criterion²⁹, which can be derived from Liapunov stability theory.

b) Distributed systems

Stability of distributed parameter systems is much more difficult to visualize than stability for lumped parameter systems. Instead of being a single point in state space, the steady state now consists of a profile which is a continuum of an infinite number of equilibrium points. Thus, the idea of phase planes becomes meaningless since a separate phase plane diagram would be needed for each of these equilibria.

Now stability depends on the proximity of the transient solution (that is, the response arising after a perturbation about the steady state profile) to the steady state profile. If the transient response remains within a finite region of the steady state the system is stable about that equilibrium profile. Asymptotic stability means that, given sufficient time, the difference between the steady state profile and the transient profile will become as small as desired. Mathematically, Liapunov stability of systems described by partial differential equations, such as

$$\frac{\partial \underline{U}}{\partial t} = \underline{f}(\underline{U})$$

is defined analogously to stability of lumped systems. Here \underline{U} , the state solution vector, is defined as a perturbation from the equilibrium vector. By making an appropriate change of coordinates the equilibrium vector can be made to coincide with the origin or null vector. Thus, the following definition is sometimes called the definition for null state stability:

DEFINITION

An equilibrium state $\underline{U}_e = \underline{0}$ is stable if for every real number $\epsilon > 0$ there exists a real number $\delta(\epsilon, t_0) > 0$ such that

$$\|\underline{U}(t_0, \underline{x})\|_{\Omega} \leq \delta(\epsilon, t_0)$$

implies that

$$\|\underline{U}(t, \underline{x})\|_{\Omega} \leq \epsilon \text{ for all } t > t_0.$$

If, in addition, $\|\underline{U}(t, \underline{x})\|_{\Omega} \rightarrow 0$ as $t \rightarrow \infty$, the null state is asymptotically stable. The notation $\|\cdot\|_{\Omega}$ denotes the effect that the dependence of $\underline{U}(t, \underline{x})$ on the position \underline{x} in the spatial domain Ω has on the norm. For example, the norm of the state vector could be taken as the L_2 norm,

$$\|\underline{U}(t, \underline{x})\|_{\Omega} = \frac{1}{2} \left[\int_{\Omega} \underline{U}^T \underline{U} d\Omega \right]^{\frac{1}{2}}$$

The most general extensions of Liapunov's work to infinite dimensional systems has been done by Zubov³⁹. He extended the previous notions concerning a Liapunov function for finite dimensional systems into the more general concept of a Liapunov functional which can be used in the infinite dimensional space. A functional is a correspondence which assigns a definite number to each function belonging to

a certain class. Zubov's main results are summarized in a theorem in Wang³².

The Liapunov stability theorem for infinite dimensional systems is a special case of Zubov's theorem. It is directly analogous to the Liapunov theorem for systems described by ordinary differential equations¹¹, that is, THEOREM¹²

The sufficient condition for a distributed parameter system to have an asymptotically stable equilibrium state is that there exists a positive-definite functional V which has a negative-definite time derivative \dot{V} along solutions to the system equations. Such a functional is called a Liapunov functional.

Just as in the simple case of the n-dimensional problem, the main problem in using the Liapunov technique in distributed parameter systems is the determination of the Liapunov functional. Zubov has suggested for a system of strongly parabolic partial differential equations that the Liapunov functional have the following form:

$$V = \frac{1}{2} \int_{\Omega} \underline{U}^T(t, \underline{x}) \underline{U}(t, \underline{x}) d\Omega$$

It is obvious that this is the distributed analog of the previous quadratic form where the matrix P has been reduced to the identity matrix I . The fact that using a weighting matrix P in the Liapunov functional yields sharper stability results will be shown in later chapters.

1.4 Methods of Determining Liapunov Stability of Distributed Parameter Systems

In the analysis of systems with distributed parameters, usually the system is first approximated by a lumped parameter model. Then known techniques for lumped systems are used⁹. Although this is a seemingly practical approach, it does not always lead to satisfactory results. For example, in the design of feedback controllers, the control law may be stable for the lumped parameter approximation, whereas, the steady states of the actual system may be unstable³³.

Hsu¹² mentions some of the problems involved with approximation with reference to the areas of nuclear reactors, heat exchangers and pneumatic transmission lines. In general, the approximations take one of the following forms³⁵.

- 1) Spatial discretization: This results in a finite system of continuous time ordinary differential equations.
- 2) Time discretization: The resulting model consists of a finite-dimensional system of spatially continuous ordinary differential equations.
- 3) Space-time discretization: The model takes the form of a finite-dimensional system of difference equations. This form is useful

for digital computation.

- 4) Spatial harmonic truncation: In cases where the state functions, over a finite spatial domain, have a band-limited spectrum with high-frequency spatial harmonics attenuated, the system may be approximated by a finite-dimensional system by truncating the spatial harmonics at a suitable frequency.

In many cases, however, the inherent distributed nature of a problem is lost by making approximating assumptions about the behavior of the system variables. For example, problems involving epidemics². It is obvious that the epidemics are distributed over a spatial domain and, although they have been modelled as partial differential equations, in some instances the assumption is made that the epidemic is isolated in such a way that no spatial dependence arises. Since the resulting model is highly unrealistic, its use could easily yield misleading conclusions.

To avoid problems involved with the various types of approximation, it is desirable for studying stability to formulate the problem directly as a distributed mathematical model^{33,36}. The distributed models involve integral and partial differential equations which, in general, are very difficult to solve. The best single technique

currently available for tackling these problems is Liapunov's direct method which has been very useful in qualitatively describing their behavior without having to solve them^{10,33}.

1.5 Scope of the Thesis

In this thesis, stability of distributed parameter systems is studied using Liapunov's second or direct method. Two techniques are presented for finding Liapunov functionals for processes which are described by systems of nonlinear partial differential equations. The first technique involves an extension to the work done by Berger and Lapidus⁴ which uses a matrix quadratic form in the integrand of the Liapunov functional. This method was suggested but not attempted by Berger and Lapidus. Two applications are provided to illustrate the technique developed. The technique is first applied to the catalyst particle problem and then to the tubular reactor problem. These two problems are characterized by the possibility of having multiple steady states.

The second technique developed is completely analogous to the well-known variable gradient method. This method has found wide use in studying stability of systems of ordinary differential equations. An algorithm is developed which extends the theory to the distributed parameter case. For the purpose of comparison, the same examples treated by the other technique are used to illustrate the variable gradient method.

CHAPTER 2

LIAPONOV STABILITY USING A
FUNCTIONAL OF QUADRATIC FORM

2.1 Introduction

In this chapter a technique is developed for determining stability of distributed parameter systems which uses a Liapunov functional having a quadratic form as the integrand²¹. In general, the problems which can be treated by this method have system equations of the following form:

$$\frac{\partial \underline{U}(t, \underline{x})}{\partial t} = \underline{f}[\underline{U}(t, \underline{x})] \quad (2.1)$$

where $\underline{U}(t, \underline{x})$ is the perturbation vector and \underline{f} , in general, represents a second-order vector nonlinear differential operator over the spatial domain. As mentioned, the Liapunov functional has the form:

$$V = \int_{\Omega} \underline{U}^T \underline{P} \underline{U} d\Omega \quad (2.2)$$

where \underline{P} is a positive-definite, symmetric matrix.

This method is an extension of the work of Berger and Lapidus⁴. Although they suggested the use of the non-identity matrix \underline{P} , they never attempted it. The development of the method will be illustrated through two examples since the details will be made clearer than by speaking in general terms. The two examples are the same as those treated by Berger and Lapidus and, therefore, the

analysis roughly parallels theirs.

2.2 Catalyst Particle Problem

Multiple steady states sometimes result when a first-order chemical reaction occurs inside a porous catalyst particle in the presence of heat and mass diffusion. A physical interpretation of these multiple equilibria may be obtained from the following diagram from Weisz and Hicks³⁷. The curved line in the sketch

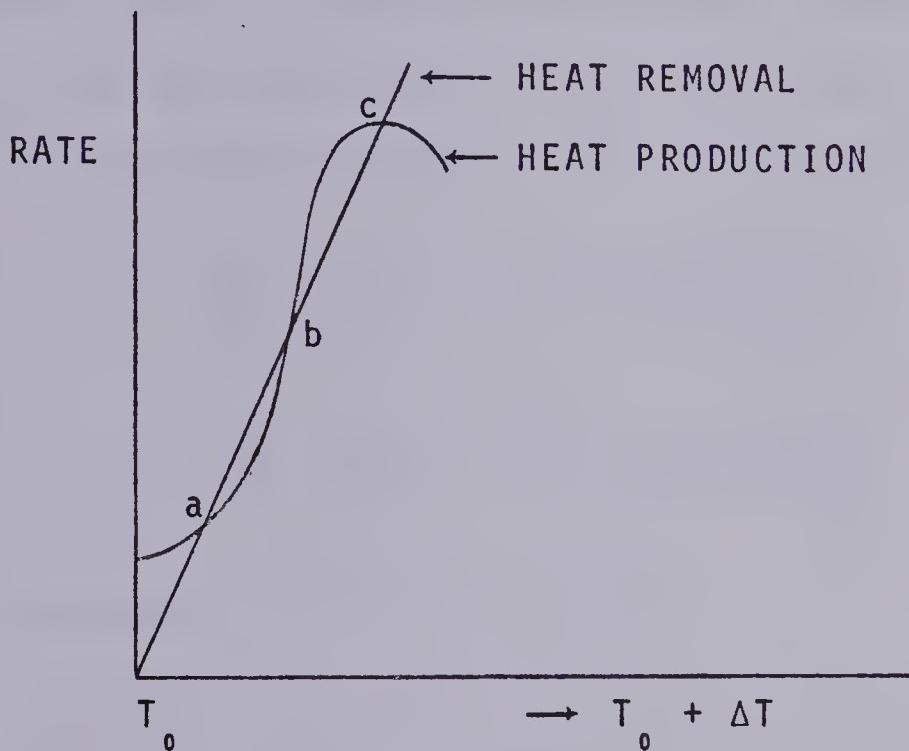


Figure 1

illustrates the functional relationship between the rate of heat production with temperature. The straight line, representing the rate of heat removal by conduction for a given temperature differential between adjoining volume elements, intersects the curve up to three times. Thus, equating heat removal and production rates results in up to three steady state solutions.

The point b is metastable. An initial temperature

condition below b results in stabilization at point a, and initial conditions corresponding to a point above b sends the system to condition c. Thus, in observing reaction rates as a function of rising temperature, a discontinuous temperature change may obtain when a metastable condition "is passed".

MATH MODEL

For the purpose of analysis, the catalyst particle is assumed to be in the form of a slab. The following dimensionless mass and heat balance equations are associated with the first-order reaction within the particle.

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial x^2} - \phi^2 y \exp \left[\frac{\gamma(z-1)}{z} \right] \quad (2.3)$$

$$N \frac{\partial z}{\partial t} = \frac{\partial^2 z}{\partial x^2} + \beta \phi^2 y \exp \left[\frac{\gamma(z-1)}{z} \right] \quad (2.4)$$

with the boundary conditions given by

$$\frac{\partial y(t,0)}{\partial x} = \frac{\partial z(t,0)}{\partial x} = 0, \quad y(t,1) = z(t,1) = 1 \quad (2.5)$$

The usual symbols are used here and their meanings are stated in the List of Symbols on page iv. The detailed derivation of these equations can be found in APPENDIX 2.

At steady state, equations (2.3) and (2.4) hold but with the time derivatives becoming zero. Denoting the solutions of the resulting steady state equations by y^* and z^* , an adiabatic balance at this equilibrium condition yields

$$z^* = 1 + \beta(1-y^*) \quad (2.6)$$

To analyse the stability about the equilibrium states, define the following set of perturbation equations by letting

$$\begin{aligned} y &= y^* + u \\ z &= z^* + v \end{aligned} \quad (2.7)$$

and, writing the nonlinear reaction rate term as

$$f(y, z) = \phi^2 y \exp\left[\frac{\gamma(z-1)}{z}\right] \quad (2.8)$$

then, (2.3) and (2.4) yield, respectively

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - f(y, z) + \frac{\partial^2 y^*}{\partial x^2} \quad (2.9)$$

$$N \frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + \beta f(y, z) + \frac{\partial^2 z^*}{\partial x^2} \quad (2.10)$$

with the boundary conditions becoming

$$\frac{\partial u(t, 0)}{\partial x} = \frac{\partial v(t, 0)}{\partial x} = u(t, 1) = v(t, 1) = 0 \quad (2.11)$$

Linearizing the nonlinear reaction rate term about the steady state profile with

$$\begin{aligned} f(y, z) &= f(y^*, z^*) + \frac{\partial f(y, z)}{\partial y} \Bigg|_{\substack{y=y^* \\ z=z^*}} u + \frac{\partial f(y, z)}{\partial z} \Bigg|_{\substack{y=y^* \\ z=z^*}} v \\ &= f(y^*) + f_y u + f_z v \end{aligned} \quad (2.12)$$

and using the steady state equations

$$\frac{\partial^2 y^*}{\partial x^2} = f(y^*) \quad (2.13)$$

$$\frac{\partial^2 z^*}{\partial x^2} = -\beta f(y^*) \quad (2.14)$$

yields the following linearized perturbation equations

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - f_y u - f_z v \quad (2.15)$$

$$\frac{\partial v}{\partial t} = M \frac{\partial^2 v}{\partial x^2} + M\beta f_y u + M\beta f_z v \quad (2.16)$$

where, for convenience, M denotes $1/N$.

Guided by the suggestions of Zubov for strongly parabolic equations, Berger and Lapidus use the following Liapunov functional

$$V = \frac{1}{2} \int_{\Omega} \underline{U}^T(t, \underline{x}) \underline{U}(t, \underline{x}) d\Omega \quad (2.17)$$

where

$$\underline{U} = [u \ v]^T, \quad (2.18)$$

the state vector. In this case (2.17) becomes

$$V = \frac{1}{2} \int_{\Omega} (u^2 + v^2) dx \quad (2.19)$$

As pointed out at the outset, the purpose of this chapter is to investigate the use of a non-identity matrix in the Liapunov functional. For this problem, equation (2.2) takes the following form

$$V = \frac{1}{2} \int_0^1 \underline{U}^T(t, x) \underline{P} \underline{U}(t, x) dx \quad (2.20)$$

P is a positive-definite symmetric matrix, written for convenience as

$$\underline{P} = \begin{bmatrix} p_1 & p_3 \\ p_3 & p_2 \end{bmatrix} \quad (2.21)$$

Expanding (2.20) with (2.18) and (2.21) yields

$$V = \frac{1}{2} \int_0^1 (p_1 u^2 + 2p_3 uv + p_2 v^2) dx \quad (2.22)$$

Since P is positive-definite, V is positive-definite.

From (2.22)

$$\dot{V} = \int_0^1 [p_1 u \frac{\partial u}{\partial t} + p_3 (u \frac{\partial v}{\partial t} + v \frac{\partial u}{\partial t}) + p_2 v \frac{\partial v}{\partial t}] dx \quad (2.23)$$

Substituting (2.15) and (2.16), (2.23) becomes

$$\begin{aligned} \dot{V} = \int_0^1 & \left(p_1 u \frac{\partial^2 u}{\partial x^2} - p_1 u^2 f_y - p_1 u v f_z \right. \\ & + p_3 M u \frac{\partial^2 v}{\partial x^2} + p_3 M \beta u^2 f_y + p_3 M \beta u v f_z \\ & + p_3 v \frac{\partial^2 u}{\partial x^2} - p_3 u v f_y - p_3 v^2 f_z \\ & \left. + p_2 M v \frac{\partial^2 v}{\partial x^2} + p_2 M \beta u v f_y + p_2 M \beta v^2 f_z \right) dx \quad (2.24) \end{aligned}$$

Using integration by parts on second-order terms, (2.24)

becomes

$$\begin{aligned} \dot{V} = \int_0^1 & \left(-p_1 \left(\frac{\partial u}{\partial x} \right)^2 - p_1 u^2 f_y - p_1 u v f_z \right. \\ & - p_3 M \left(\frac{\partial u}{\partial x} \right) \left(\frac{\partial v}{\partial x} \right) + p_3 M \beta u^2 f_y + p_3 M \beta u v f_z \\ & - p_3 \left(\frac{\partial u}{\partial x} \right) \left(\frac{\partial v}{\partial x} \right) - p_3 u v f_y - p_3 v^2 f_z \\ & \left. - p_2 M \left(\frac{\partial v}{\partial x} \right)^2 + p_2 M \beta u v f_y + p_2 M \beta v^2 f_z \right) dx \quad (2.25) \end{aligned}$$

Consider the following inequality

$$0 \leq (m \pm n)^2 = m^2 \pm 2mn + n^2$$

Thus $\pm 2mn \leq m^2 + n^2$

or, in general

$$\pm amn \leq |a| |mn| \leq \left| \frac{a}{2} \right| (m^2 + n^2) \quad (2.26)$$

Using (2.26) in (2.25) and rearranging yields

$$\begin{aligned} \dot{v} &\leq \int_0^1 u^2 (p_3 M\beta f_y - p_1 f_y + \frac{1}{2} |p_3 M\beta f_z - p_1 f_z - p_3 f_y + p_2 M\beta f_y|) dx \\ &+ \int_0^1 v^2 (p_2 M\beta f_z - p_3 f_z + \frac{1}{2} |p_3 M\beta f_z - p_1 f_z - p_3 f_y + p_2 M\beta f_y|) dx \\ &+ \int_0^1 (\frac{\partial u}{\partial x})^2 (-p_1 + \frac{1}{2} |p_3 (M+1)|) dx \\ &+ \int_0^1 (\frac{\partial v}{\partial x})^2 (-p_2 M + \frac{1}{2} |p_3 (M+1)|) dx \end{aligned} \quad (2.27)$$

To simplify this expression let

$$F_u = (p_3 M\beta - p_1) f_y + \frac{1}{2} |(p_3 M\beta - p_1) f_z + (p_2 M\beta - p_3) f_y| \quad (2.28)$$

$$F_v = (p_2 M\beta - p_3) f_z + \frac{1}{2} |(p_3 M\beta - p_1) f_z + (p_2 M\beta - p_3) f_y| \quad (2.29)$$

Then (2.27) becomes

$$\begin{aligned} \dot{v} &\leq \int_0^1 u^2 F_u dx + \int_0^1 v^2 F_v dx \\ &- \int_0^1 (\frac{\partial u}{\partial x})^2 (p_1 - \frac{1}{2}(M+1) |p_3|) dx \\ &- \int_0^1 (\frac{\partial v}{\partial x})^2 (p_2 M - \frac{1}{2}(M+1) |p_3|) dx \end{aligned} \quad (2.30)$$

Now consider an inequality credited to Gavalas⁸. From the

identity

$$u(t,x) = - \int_x^1 \frac{\partial u}{\partial x}(t,x) dx, \text{ for } u(t,1)=0$$

it follows that

$$u^2(t,x) = \left(\int_x^1 \frac{\partial u}{\partial x}(t,x) dx \right)^2$$

and with the Schwarz inequality³¹

$$\begin{aligned} u^2(t,x) &\leq \int_x^1 \left(\frac{\partial u}{\partial x} \right)^2 dx \int_x^1 (1)^2 dx \\ \text{or } u^2(t,x) &\leq (1-x) \int_x^1 \left(\frac{\partial u}{\partial x} \right)^2 dx \end{aligned} \quad (2.31)$$

Similarly

$$v^2(t,x) \leq (1-x) \int_x^1 \left(\frac{\partial v}{\partial x} \right)^2 dx \quad (2.32)$$

With (2.31) and (2.32) equation (2.30) can be written

$$\begin{aligned} \dot{v} &\leq \int_0^1 F_u \left[(1-x) \int_0^1 \left(\frac{\partial u}{\partial x} \right)^2 dx \right] dx \\ &+ \int_0^1 F_v \left[(1-x) \int_0^1 \left(\frac{\partial v}{\partial x} \right)^2 dx \right] dx \\ &- \int_0^1 \left(\frac{\partial u}{\partial x} \right)^2 \left[p_1 - \frac{1}{2}(M+1)|p_3| \right] dx \\ &- \int_0^1 \left(\frac{\partial v}{\partial x} \right)^2 \left[p_2 M - \frac{1}{2}(M+1)|p_3| \right] dx \end{aligned} \quad (2.33)$$

rearranging finally yields

$$\begin{aligned} \dot{v} &\leq \left(\int_0^1 \left(\frac{\partial u}{\partial x} \right)^2 dx \right) \left(-\{p_1 - \frac{1}{2}(M+1)|p_3|\} + \int_0^1 (1-x) F_u dx \right) \\ &+ \left(\int_0^1 \left(\frac{\partial v}{\partial x} \right)^2 dx \right) \left(-\{p_2 M - \frac{1}{2}(M+1)|p_3|\} + \int_0^1 (1-x) F_v dx \right) \end{aligned} \quad (2.34)$$

It is apparent from (2.34) that two criteria must hold simultaneously to give a sufficient condition for asymptotic stability. These criteria are

$$(a) \int_0^1 (1-x) F_u \, dx < p_1 - \frac{1}{2}(M+1)|p_3| \quad (2.35)$$

$$(b) \int_0^1 (1-x) F_v \, dx < p_2 M - \frac{1}{2}(M+1)|p_3| \quad (2.36)$$

DISCUSSION AND RESULTS

The derivation here differs slightly from the work of Berger and Lapidus. They separated the integral of F_u into two sets corresponding to intervals where $F_u > 0$ and intervals where $F_u < 0$. The integral of F_v was not similarly manipulated, since, in their case $P = I$, the identity matrix, and thus, $F_v > 0$ for $0 \leq x \leq 1$. For their special case of $N=1$, in place of (2.30) they obtained

$$\begin{aligned} \dot{V} \leq & - \int_0^1 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 \right] dx + \int_0^1 v^2 F_v \, dx \\ & + \int_{\alpha''}^{\beta''} |F_u| u^2 \, dx - \int_{\substack{x \notin [\alpha'', \beta''] \\ x \in [0, 1]}} |F_u| u^2 \, dx \end{aligned} \quad (2.37)$$

In the next step Berger and Lapidus throw out the last term for no apparent reason except that it strengthens the inequality.

As will be shown the retention of all terms in (2.30) is advisable when a weighting matrix is used in the Liapunov functional. It was found that both F_u and F_v could

oscillate from positive to negative with x and that restricting x to only those intervals where the functions were positive resulted in cases from which no conclusion about stability could be drawn. However, for the same cases retention of all terms, that is, not restricting x , allowed conclusions of asymptotic stability to be made.

The sufficient conditions for asymptotic stability which result from restricting x to only those intervals where $F_u > 0$ and $F_v > 0$ are

$$(a)' \int_{F_u > 0} (1-x) F_u \, dx < p_1 - \frac{1}{2}(M+1)|p_3| \quad (2.38)$$

$$(b)' \int_{F_v > 0} (1-x) F_v \, dx < p_2 M - \frac{1}{2}(M+1)|p_3| \quad (2.39)$$

It is obvious from the two sets of sufficient conditions (2.35), (2.36) and (2.38), (2.39) that the first set would be the easier to satisfy. For example, split up the left hand term in (2.35) and compare it to the left hand term in (2.38). That is, compare

$$\int_0^1 (1-x) F_u \, dx = \int_{F_u > 0} (1-x) F_u \, dx - \int_{F_u < 0} (1-x) |F_u| \, dx$$

with just

$$\int_{F_u > 0} (1-x) F_u \, dx$$

Thus, in trying to satisfy the respective sufficient conditions for asymptotic stability it will be more difficult in the case of condition (a)' since the left

hand side has lost a term which tends to reduce its magnitude while the right sides remain unchanged.

As mentioned previously, this system has three possible steady states, two of which should be stable and one metastable. By using the analysis outlined above for the special case of $N=1$, Berger and Lapidus were able to conclude only that the first steady state is asymptotically stable. By using a weighting matrix and by retaining all terms of inequality (2.30) both steady states one and three were shown to be stable for various values of N . Some of the results are shown in table 1 along with the results of Berger and Lapidus. In all values of N , one result is shown where dropping the above-mentioned terms yields no conclusion about stability.

The IBM/APL 360/67 computer system with direct access time sharing facilities was extremely efficient for handling the computations required for this problem. Although suitable elements of the matrix \underline{P} can be found only by trial and error methods, the APL system made this task straight-forward.

As the identity matrix enabled stability conclusions to be made for steady state one for most values of N , it was always used as an initial trial for each steady state. Then, if that failed to produce a conclusion about stability, the following general procedure was implemented.

TABLE 1

N	<u>P</u> MATRIX	STEADY STATE #	CONDITION (a)		CONDITION (b)		COMMENT
			L.H.S.	R.H.S.	L.H.S.	R.H.S.	
1	1 1 0	1	0.1272	1	0.3494	1	Stable
	1 2 1.4	1	0.0030	-0.4	0.0048	0.6	No conclusion
	1 1 0	2	1.724	1	6.037	1	No conclusion
	1 2 1.4	2	0.0439	-0.4	0.0835	0.6	No conclusion
	1 1 0	3	-25.87	1	17.29	1	No conclusion
	1 2 1.4	3	-0.7649	-0.4	0.1471	0.6	Stable
	1 2 1.4	3	0.0074	-0.4	0.1471	0.6	No conclusion*
	1 1 0	1	0.1300	1	0.2486	0.5	Stable
	1 5.7 2	1	0.0398	-0.5	0.0429	1.35	No conclusion
	1 1 0	2	1.839	1	4.324	0.5	No conclusion
2	1 5.7 2	2	0.5877	-0.5	0.7589	1.35	No conclusion
	1 1 0	3	-31.07	1	9.328	0.5	No conclusion
	1 5.7 2	3	-10.01	-0.5	1.239	1.35	Stable
	1 5.7 2	3	0.1137	-0.5	1.239	1.35	No conclusion*

* These values were obtained using conditions (a)' and (b)'.

Without loss of generality, let $p_1 = 1$. The values of p_2 and p_3 are then chosen arbitrarily, keeping in mind that \underline{P} must be positive-definite. Inequalities (2.35) and (2.36) are tested. If they are not satisfied, the value of p_2 (or p_3) is changed and the tests are repeated. If the tests fail again one can compare the amounts by which the inequalities failed to be satisfied and use these amounts to immediately determine whether the direction of the change chosen for p_2 (or p_3) was correct. That is, if the inequality held in reverse, the amount by which the left hand side exceeded the right hand side serves as a measure of convergence or lack of convergence toward a satisfactory \underline{P} matrix. It was sometimes necessary to also vary the third element to finally arrive at such a matrix.

2.3 Tubular Reactor Problem

In this section the method developed earlier is further illustrated by means of a second example. A simple first-order chemical reaction which takes place in a tubular reactor is analysed to determine the stability of the steady states. The fluid in the reactor is assumed to be in turbulent flow such that radial effects may be neglected. Thus, the only diffusion which occurs is in the axial direction.

MATH MODEL

The normalized mass and heat balance equations are

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial s^2} - N_p \frac{\partial y}{\partial s} + \alpha y \exp(-Q/z) \quad (2.40)$$

$$\frac{\partial z}{\partial t} = \frac{\partial^2 z}{\partial s^2} - N_p \frac{\partial z}{\partial s} + \nu y \exp(-Q/z) \quad (2.41)$$

with

$$N_p(1-y(t,0)) = - \frac{\partial y}{\partial s}(t,0), \quad \frac{\partial y}{\partial s}(t,1) = 0 \quad (2.42)$$

$$N_p(1-z(t,0)) = - \frac{\partial z}{\partial s}(t,0), \quad \frac{\partial z}{\partial s}(t,1) = 0$$

where, again, the symbols are as defined in the List of Symbols on page iv.

As in section 2.2, generalized perturbation is used here to determine the stability of the steady states. These generalized results are later reduced to the special case of the adiabatic perturbation and the results so obtained are compared to those in⁴.

Consider the nonlinear term

$$f(y, z) = y \exp(-Q/z) \quad (2.43)$$

Linearizing this about the steady state y^*, z^* yields

$$f(y, z) = f(y^*, z^*) + \left. \frac{\partial f}{\partial y} \right|_{\substack{y=y^* \\ z=z^*}} (y - y^*) + \left. \frac{\partial f}{\partial z} \right|_{\substack{y=y^* \\ z=z^*}} (z - z^*) \quad (2.44)$$

At steady state, (2.40) and (2.41) become

$$\frac{\partial^2 y^*}{\partial s^2} = N_p \frac{\partial y^*}{\partial s} - \alpha f(y^*, z^*) \quad (2.45)$$

$$\frac{\partial^2 z^*}{\partial s^2} = N_p \frac{\partial z^*}{\partial s} - \nu f(y^*, z^*) \quad (2.46)$$

So, if the perturbations in y and z are denoted as before by u and v , respectively, the transient equations can be written as

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial s^2} - N_p \frac{\partial u}{\partial s} + \frac{\partial^2 y^*}{\partial s^2} - N_p \frac{\partial y^*}{\partial s} + \alpha f(y^*, z^*) + \alpha f_y u + \alpha f_z v \quad (2.47)$$

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial s^2} - N_p \frac{\partial v}{\partial s} + \frac{\partial^2 z^*}{\partial s^2} - N_p \frac{\partial z^*}{\partial s} + v f(y^*, z^*) + v f_y u + v f_z v \quad (2.48)$$

combining the last four equations yields

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial s^2} - N_p \frac{\partial u}{\partial s} + \alpha f_y u + \alpha f_z v \quad (2.49)$$

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial s^2} - N_p \frac{\partial v}{\partial s} + v f_y u + v f_z v \quad (2.50)$$

with the boundary conditions

$$u(t, 0) = v(t, 0) = 0 \text{ (assumed)} \quad (2.51)$$

and $\frac{\partial u(t, 1)}{\partial s} = \frac{\partial v(t, 1)}{\partial s} = 0$ (from (2.42))

To make analysis easier, the following transformations will be used

$$u(t, s) = \xi(t, s) \exp\left[\frac{N_p s}{2}\right] \quad (2.52)$$

$$v(t, s) = \eta(t, s) \exp\left[\frac{N_p s}{2}\right] \quad (2.53)$$

These relations transform (2.49) and (2.50) into the following

$$\frac{\partial \xi}{\partial t} = \frac{\partial^2 \xi}{\partial s^2} + \xi \left[\alpha f_y - \frac{N_p^2}{4} \right] + \alpha n f_z \quad (2.54)$$

$$\frac{\partial \eta}{\partial t} = \frac{\partial^2 \eta}{\partial s^2} + \eta \left[v f_z - \frac{N_p^2}{4} \right] + v \xi f_y \quad (2.55)$$

with the boundary conditions

$$\begin{aligned}\xi(t,0) &= \eta(t,0) = 0 \\ \frac{\partial \xi}{\partial s}(t,1) &= -\frac{N_p}{2} \xi(t,1) \\ \frac{\partial \eta}{\partial s}(t,1) &= -\frac{N_p}{2} \eta(t,1)\end{aligned}\quad (2.56)$$

As in section 2.2, let

$$v = \frac{1}{2} \int_0^1 \underline{U}^T(t,s) \underline{P} \underline{U}(t,s) ds \quad (2.57)$$

where

$$\underline{U} = \begin{bmatrix} \xi(t,s) \\ \eta(t,s) \end{bmatrix}$$

and, as before

$$\underline{P} = \begin{bmatrix} p_1 & p_3 \\ p_3 & p_2 \end{bmatrix}$$

Differentiating (2.57) with respect to time yields

$$\dot{v} = \int_0^1 [p_1 \xi \frac{\partial \xi}{\partial t} + p_3 (\xi \frac{\partial \eta}{\partial t} + \eta \frac{\partial \xi}{\partial t}) + p_2 \eta \frac{\partial \eta}{\partial t}] ds \quad (2.58)$$

Substituting (2.54) and (2.55) into (2.58) yields

$$\begin{aligned}\dot{v} &= \int_0^1 \left[p_1 \xi \left\{ \frac{\partial^2 \xi}{\partial s^2} - \frac{N^2}{4} p \xi + \alpha \xi f_y + \alpha n f_z \right\} \right. \\ &\quad + p_3 \left(\xi \left\{ \frac{\partial^2 \eta}{\partial s^2} - \frac{N^2}{4} p \eta + v \xi f_y + v n f_z \right\} \right. \\ &\quad + \eta \left\{ \frac{\partial^2 \xi}{\partial s^2} - \frac{N^2}{4} p \xi + \alpha \xi f_y + \alpha n f_z \right\} \Big) \\ &\quad \left. + p_2 \eta \left\{ \frac{\partial^2 \eta}{\partial s^2} - \frac{N^2}{4} p \eta + v \xi f_y + v n f_z \right\} \right] ds \quad (2.59)\end{aligned}$$

Integration by parts of some of the terms in (2.59) yields the following

$$\begin{aligned} \int_0^1 \xi \frac{\partial^2 \xi}{\partial s^2} ds &= \xi \frac{\partial \xi}{\partial s} \Big|_0^1 - \int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds \\ &= \xi(t, 1) \frac{\partial \xi}{\partial s}(t, 1) - \int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds \\ &= -\frac{N_p}{2} \xi^2(t, 1) - \int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds \end{aligned} \quad (2.60)$$

Similarly

$$\int_0^1 \eta \frac{\partial^2 \eta}{\partial s^2} ds = -\frac{N_p}{2} \eta^2(t, 1) - \int_0^1 \left(\frac{\partial \eta}{\partial s} \right)^2 ds \quad (2.61)$$

also

$$\begin{aligned} \int_0^1 \eta \frac{\partial^2 \xi}{\partial s^2} ds &= \int_0^1 \xi \frac{\partial^2 \eta}{\partial s^2} ds \\ &= -\frac{N_p}{2} \xi(t, 1) \eta(t, 1) - \int_0^1 \left(\frac{\partial \xi}{\partial s} \right) \left(\frac{\partial \eta}{\partial s} \right) ds \end{aligned} \quad (2.62)$$

Equation (2.59) can now be written

$$\begin{aligned} \dot{v} &= -p_1 \frac{N_p}{2} \xi^2(t, 1) - p_3 N_p \xi(t, 1) \eta(t, 1) - p_2 \frac{N_p}{2} \eta^2(t, 1) \\ &\quad - p_1 \int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds - p_2 \int_0^1 \left(\frac{\partial \eta}{\partial s} \right)^2 ds - 2p_3 \int_0^1 \left(\frac{\partial \xi}{\partial s} \right) \left(\frac{\partial \eta}{\partial s} \right) ds \\ &\quad + \int_0^1 \xi^2 \left[p_1 (\alpha f_y - \frac{N_p}{4}) + p_3 v f_y \right] ds \\ &\quad + \int_0^1 \eta^2 \left[p_2 (v f_z - \frac{N_p}{4}) + p_3 \alpha f_z \right] ds \\ &\quad + \int_0^1 \xi \eta \left[p_1 \alpha f_z + p_3 (v f_z - \frac{N_p}{2} + \alpha f_y) + p_2 v f_y \right] ds \end{aligned} \quad (2.63)$$

Consider the following equality

$$\xi(t, s) = \int_0^s \left(\frac{\partial \xi}{\partial s} \right) ds$$

therefore

$$\xi^2(t,s) = \left(\int_0^s \left(\frac{\partial \xi}{\partial s} \right)^2 ds \right)^2 \quad (2.64)$$

Now, with Schwarz's inequality

$$\begin{aligned} \xi^2(t,s) &\leq \left(\int_0^s (1)^2 ds \right) \left(\int_0^s \left(\frac{\partial \xi}{\partial s} \right)^2 ds \right) \\ &\leq s \int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds \end{aligned} \quad (2.65)$$

Similarly

$$\eta^2(t,s) \leq s \int_0^1 \left(\frac{\partial \eta}{\partial s} \right)^2 ds \quad (2.66)$$

The product term can be handled using the inequality used in section 2.2, that is

$$\pm a \xi \eta \leq |a| |\xi \eta| \leq \frac{|a| (\xi^2 + \eta^2)}{2} \quad (2.67)$$

Upon substitution of (2.56), (2.66) and (2.67) into

(2.63) yields

$$\begin{aligned} \dot{v} &\leq - p_1 \frac{N_p}{2} \xi^2(t,1) - p_2 \frac{N_p}{2} \eta^2(t,1) - p_3 N_p \xi(t,1) \eta(t,1) \\ &+ \left(\int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds \right) \left(- p_1 + \int_0^1 s p_1 (\alpha f_y - \frac{N_p}{4}) + p_3 v f_y ds \right. \\ &+ 2 |p_3| + \int_0^1 \frac{s}{2} |p_1 \alpha f_z + p_3 (v f_z - \frac{N_p}{2} + \alpha f_y) + p_2 v f_y| ds \Big) \\ &+ \left(\int_0^1 \left(\frac{\partial \eta}{\partial s} \right)^2 ds \right) \left(- p_2 + \int_0^1 s p_2 (v f_z - \frac{N_p}{4}) + p_3 \alpha f_z ds \right. \\ &+ 2 |p_3| + \int_0^1 \frac{s}{2} |p_1 \alpha f_z + p_3 (v f_z - \frac{N_p}{2} + \alpha f_y) + p_2 v f_y| ds \Big) \end{aligned} \quad (2.68)$$

To simplify this expression, let

$$\begin{aligned} F_\xi &= p_1 (\alpha f_y - \frac{N_p}{4}) + p_3 v f_y \\ &\quad + \frac{1}{2} |p_1 \alpha f_z + p_3 (v f_z - \frac{N_p}{2} + \alpha f_y) + p_2 v f_y| \quad (2.69) \end{aligned}$$

and

$$\begin{aligned} F_\eta &= p_2 (v f_z - \frac{N_p}{4}) + p_3 \alpha f_z \\ &\quad + \frac{1}{2} |p_1 \alpha f_z + p_3 (v f_z - \frac{N_p}{2} + \alpha f_y) + p_2 v f_y| \quad (2.70) \end{aligned}$$

Then

$$\begin{aligned} \dot{V} &\leq - p_1 \frac{N_p}{2} \xi^2(t, 1) - p_2 \frac{N_p}{2} \eta^2(t, 1) - p_3 N_p \xi(t, 1) \eta(t, 1) \\ &\quad + \left(\int_0^1 \left(\frac{\partial \xi}{\partial s} \right)^2 ds \right) \left(- p_1 + 2|p_3| + \int_0^1 s F_\xi ds \right) \\ &\quad + \left(\int_0^1 \left(\frac{\partial \eta}{\partial s} \right)^2 ds \right) \left(- p_2 + 2|p_3| + \int_0^1 s F_\eta ds \right) \quad (2.71) \end{aligned}$$

Consider only the first three terms of (2.71)

$$\begin{aligned} - \frac{N_p}{2} p_1 \xi^2(t, 1) - N_p p_3 \xi(t, 1) \eta(t, 1) - p_2 \frac{N_p}{2} \eta^2(t, 1) \\ = - \frac{N_p}{2} p_1 \left[\xi^2(t, 1) + 2 \frac{p_3}{p_1} \xi(t, 1) \eta(t, 1) + \frac{p_2}{p_1} \eta^2(t, 1) \right] \quad (2.72) \end{aligned}$$

Since matrix \underline{P} is positive-definite,

$$p_1 p_2 - p_3^2 > 0 \text{ and } p_1 > 0$$

Hence

$$p_3 < +\sqrt{p_1 p_2}$$

$$- p_3 < +\sqrt{p_1 p_2} \quad (2.73)$$

By (2.73), the terms in (2.72) can be written

$$\begin{aligned}
 & -\frac{N_p}{2} p_1 \xi^2(t,1) - N_p p_3 \xi(t,1) n(t,1) - p_2 \frac{N_p}{2} n^2(t,1) \\
 & < -\frac{N_p}{2} p_1 \left(\xi(t,1) - \frac{\sqrt{p_2}}{\sqrt{p_1}} n(t,1) \right)^2
 \end{aligned} \tag{2.74}$$

And, since $N_p > 0$, it is clear that the first three terms of (2.71) are negative-definite. Hence, in order for $\dot{V} < 0$, the following conditions are sufficient

$$\int_0^1 s F_\xi \, ds < p_1 - 2|p_3| \tag{2.75}$$

$$\int_0^1 s F_n \, ds < p_2 - 2|p_3| \tag{2.76}$$

For the special case of adiabatic perturbation, the following relation holds

$$\beta \xi = -n \tag{2.77}$$

When equation (2.77) is used in (2.71), the following sufficient condition for asymptotic stability is obtained

$$\int_0^1 s \left(\frac{F_\xi}{\beta^2} + F_n \right) ds < \frac{p_1}{\beta^2} + p_2 - 2|p_3| \left(\frac{\beta^2 + 1}{\beta^2} \right) \tag{2.78}$$

DISCUSSION AND RESULTS

In solving for the steady state profiles the following parameter values were used

$$\beta = 0.40, N = 30, Q = 30 \text{ and } \alpha = 2.25 \times 10^{13}$$

which are the same values that were used in⁴. The profiles were generated on an APL/360 direct-access system* using a

*

For the specific functions used, see the APPENDIX

double precision variable step-size Runge-Kutta method.

The integration was carried out backwards toward the inlet of the reactor until the so-called Danckwert boundary condition was satisfied there. The normalized output temperatures which satisfied these input conditions are shown below

Steady state no.	Normalized output temperature
1	1.053
2	1.3166
3	1.399999

The same algorithm which was roughly outlined in the previous section was used here to find the elements of the matrix \underline{P} for both steady states 2 and 3. Steady state 1 proved to be asymptotically stable by using the identity matrix. For steady state 2 the method failed to converge to a matrix \underline{P} which would satisfy the sufficient conditions (2.75) and (2.76). Although this is not a confirmation of the fact that steady state 2 is unstable³⁷, it does show that, in this case, the method does not yield matrices which would indicate that the steady state is stable. The results are contained in Table 2.

The results for the adiabatic tubular reactor, obtained using the sufficient condition (2.78), are shown in Table 3. A comparison of these results with those in⁴ shows that the use of a non-identity matrix \underline{P} in the Liapunov functional has been successful in proving that steady states 1 and 3 are both asymptotically stable,

TABLE 2

STEADY STATE #	P p_1 p_2 p_3	MATRIX	INEQUALITY (2.75)		INEQUALITY (2.76)		COMMENT
			L.H.S.	R.H.S.	L.H.S.	R.H.S.	
1	1	1 0	-74.305	1	-49.116	1	Stable
2	1	1 0	185.06	1	287.94	1	No conclusion
3	1	1 0	1097.6	1	486.67	1	No conclusion
3	1	8 -3.5	-20.149	-6	-631.43	1	Stable

whereas, the use of an identity matrix proved only that steady state 1 is stable. Table 2 shows that the tubular reactor subjected to generalized perturbations in concentration and temperature also exhibits two asymptotically stable steady states.

TABLE 3

STEADY STATE #	<u>P</u> MATRIX			INEQUALITY (2.78)		COMMENT
	p ₁	p ₂	p ₃	L.H.S.	R.H.S.	
1	1	1	0	-513.52	7.25	Stable
2	1	1	0	1444.6	7.25	No conclusion
3	1	1	0	7346.5	7.25	No conclusion
3	1	8	-3.5	-757.37	-36.45	Stable

CHAPTER 3

VARIABLE GRADIENT METHOD FOR
CERTAIN DISTRIBUTED PARAMETER SYSTEMS3.1 Introduction

The objective of this chapter is to present a method analogous to the variable gradient method for lumped systems proposed by Schultz and Gibson⁹. This method has been applied to a few distributed parameter systems. Further work may yield successful results for other systems as well.

3.2 Variable Gradient Method For Lumped Systems

In this section, the variable gradient method as applied to systems described by ordinary differential equations will be briefly reviewed. The purpose of this review is two-fold: One, to make the thesis somewhat self-contained and, two, to set the tone for the extension of the method to distributed parameter systems which follows.

The main difficulty in applying Liapunov's direct method has always been in finding Liapunov functions in a straightforward manner. The variable gradient method is based on the fact that if there exists a Liapunov function capable of proving asymptotic stability of a particular system, then, the gradient of this function also exists. The introduction of a variable gradient somewhat reduces the emphasis on the ingenuity and experience of the investigator. This will be clear as the discussion proceeds.

Consider the system of equations

$$\dot{\underline{R}} = \underline{f}(\underline{R}) \quad (3.1)$$

with

$$\underline{f}(\underline{0}) = \underline{0} \quad (3.2)$$

Assume a tentative Liapunov function

$$V = V(\underline{R})$$

then

$$\dot{V} = \frac{\partial V}{\partial r_1} \dot{r}_1 + \frac{\partial V}{\partial r_2} \dot{r}_2 + \cdots + \frac{\partial V}{\partial r_n} \dot{r}_n \quad (3.3)$$

or

$$\dot{V} = (\nabla V)^T \dot{\underline{R}} = \nabla V \cdot \dot{\underline{R}} \quad (3.4)$$

where

$$\begin{aligned} \nabla V &= \left[\frac{\partial V}{\partial r_1}, \frac{\partial V}{\partial r_2}, \dots, \frac{\partial V}{\partial r_n} \right]^T \\ &= [\nabla V_1, \nabla V_2, \dots, \nabla V_n]^T \end{aligned}$$

From ∇V , find V as follows

$$V = \int_{\underline{0}}^{\underline{R}} \nabla V \cdot d\underline{R} \quad (3.5)$$

If the stipulation that

$$\frac{\partial(\nabla V_i)}{\partial r_j} = \frac{\partial(\nabla V_j)}{\partial r_i}; i, j = 1, 2, \dots, n \quad (3.6)$$

holds, then $V(\underline{R})$ is independent of the path of integration.

Choose the simplest path as follows

$$\begin{aligned} V(\underline{R}) &= \int_0^{r_1} \nabla V_1(u_1, 0, \dots, 0) du_1 \\ &\quad + \int_0^{r_2} \nabla V_2(r_1, u_2, 0, \dots, 0) du_2 + \dots \\ &\quad + \int_0^{r_n} \nabla V_n(r_1, r_2, \dots, r_{n-1}, u_n) du_n \end{aligned} \quad (3.7)$$

Thus, the problem of determining a Liapunov function which satisfies Liapunov's theorem has been transformed into the problem of determining the gradient of V such that condition (3.6) holds.

The following procedure is used to evaluate the Liapunov function.

1. Assume an arbitrary column vector for $\underline{\nabla}V$ such as

$$\underline{\nabla}V = \begin{bmatrix} a_{11}r_1 + a_{12}r_2 + \dots + a_{1n}r_n \\ \vdots \\ \vdots \\ a_{1r_1} + a_{2r_2} + \dots + a_{nr_n} \end{bmatrix} \quad (3.8)$$

The a_{ij} 's, in general, consist of a constant part and a variable part which is a function of the state variables.

Without loss of generality, a_{ij} variable parts are functions only of r_i except for a_{nn} which is only a constant (usually 2) to simplify the proof that $V(\underline{R}) = C$ (a constant) represents closed surfaces⁷.

2. Determine \dot{V} from $\underline{\nabla}V$ by (3.4).

3. Constrain \dot{V} to be at least negative semi-definite

4. Set $a_{nn} = \text{constant}$, as above, and determine the remaining a_{ij} by using relation (3.6).

5. Recheck \dot{V} to be sure that step 4 has not altered the constraints of step 3.

6. Determine V from equation (3.7).

3.3 Extension of the Variable Gradient Method
to Distributed Parameter Systems

In the case of distributed parameter systems the Liapunov function becomes a Liapunov functional. Now the vector system equation has the form

$$\frac{\partial \underline{R}}{\partial t} = \underline{f}(t, \underline{R}) \quad (3.9)$$

since $\underline{R} = \underline{R}(t, x)$

where x is the spatial variable (in the one-dimensional case).

Now, if we assume the existence of a Liapunov functional V in the following form

$$V = \int_{\Omega} H d\Omega \quad (3.10)$$

where Ω represents the spatial domain. Then, differentiating with respect to time yields

$$\dot{V} = \int_{\Omega} \frac{\partial H}{\partial t} d\Omega \quad (3.11)$$

assuming that Ω is independent of time. The integrand may be written as

$$\frac{\partial H}{\partial t} = \frac{\partial H}{\partial r_1} \frac{\partial r_1}{\partial t} + \frac{\partial H}{\partial r_2} \frac{\partial r_2}{\partial t} + \dots + \frac{\partial H}{\partial r_n} \frac{\partial r_n}{\partial t} \quad (3.12)$$

or

$$\frac{\partial H}{\partial t} = (\nabla H)^T \frac{\partial \underline{R}}{\partial t} \quad (3.13)$$

Thus, if we assume an arbitrary form for ∇H it is possible to evaluate $\frac{\partial H}{\partial t}$ and H in a method similar to the one outlined earlier for lumped systems. An analogous

algorithm to use to evaluate V and \dot{V} from $\underline{\nabla}H$ might be as follows

1. Assume $\underline{\nabla}H$ has the form

$$\underline{\nabla}H = \begin{bmatrix} a_{11}r_1 + a_{12}r_2 + \dots + a_{1n}r_n \\ \vdots & \vdots & \vdots & \vdots \\ a_{11}r_1 + a_{22}r_2 + \dots + a_{nn}r_n \end{bmatrix} \quad (3.14)$$

2. $\frac{\partial H}{\partial t} = (\underline{\nabla}H)^T \frac{\partial R}{\partial t}$ (3.15)

3. Constrain $\dot{V} = \int_{\Omega} \frac{\partial H}{\partial t} d\Omega$

to be at least negative semi-definite. Do not merely constrain $\frac{\partial H}{\partial t} \leq 0$ since this would be much too restrictive.

4. As before set a_{nn} to some constant and use the following $\frac{n(n-1)}{2}$ curl equations to determine the remaining a_{ij}

$$\frac{\partial(\nabla H_i)}{\partial r_j} = \frac{\partial(\nabla H_j)}{\partial r_i} ; i, j = 1, 2, \dots, n \quad (3.16)$$

5. Recheck \dot{V} since step 4 may have altered the constraint mentioned in step 3.

6. Determine V from

$$V = \int_{\Omega} H d\Omega \quad (3.17)$$

where $H = \int_{\underline{0}}^{\underline{R}} (\underline{\nabla}H)^T d\underline{R}$

Again, the simplest path of integration is used, that is

$$\begin{aligned}
 H = & \int_0^{r_1} \nabla H_1(u_1, 0, \dots, 0) du_1 \\
 & + \int_0^{r_2} \nabla H_2(r_1, u_2, 0, \dots, 0) du_2 + \dots \\
 & + \int_0^{r_n} \nabla H_n(r_1, r_2, \dots, r_{n-1}, u_n) du_n \quad (3.18)
 \end{aligned}$$

3.4 An Example: The Catalyst Particle Problem

The method outlined above is first applied to the catalyst particle problem discussed earlier. Starting from the linearized perturbation equations (2.15) and (2.16)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - f_y u - f_z v \quad (3.19)$$

$$\frac{\partial v}{\partial t} = M \frac{\partial^2 v}{\partial x^2} + M\beta f_y u + M\beta f_z v \quad (3.20)$$

Proceed as follows:

Assume

$$\underline{\nabla H} = \begin{bmatrix} a_{11} u + a_{12} v \\ a_{21} u + 2v \end{bmatrix}$$

then

$$\frac{\partial H}{\partial t} = (\underline{\nabla H})^T \frac{\partial \underline{R}}{\partial t}$$

where $\underline{R} = [u \ v]^T$, thus

$$\begin{aligned}
 \frac{\partial H}{\partial t} = & \left[a_{11} u + a_{12} v, a_{21} u + 2v \right] \times \begin{bmatrix} \frac{\partial^2 u}{\partial x^2} - f_y u - f_z v \\ M \frac{\partial^2 v}{\partial x^2} + M\beta f_y u + M\beta f_z v \end{bmatrix} \\
 & \quad (3.21)
 \end{aligned}$$

By the curl equations, $a_{12} = a_{21}$

Combining this with (3.21) and (3.11) yields

$$\begin{aligned}\dot{v} = & \int_0^1 a_{11} u \frac{\partial^2 u}{\partial x^2} + 2Mv \frac{\partial^2 v}{\partial x^2} dx \\ & + \int_0^1 a_{12} \left(v \frac{\partial^2 u}{\partial x^2} + Mu \frac{\partial^2 v}{\partial x^2} \right) dx \\ & + \int_0^1 \left[u^2 (a_{12} M\beta f_y - a_{11} f_y) + v^2 (2M\beta f_z - a_{12} f_z) \right] dx \\ & + \int_0^1 uv \left[2M\beta f_y - a_{11} f_z + a_{12} (M\beta f_z - f_y) \right] dx \quad (3.22)\end{aligned}$$

Here again use can be made of the inequality employed in chapter 2, that is

$$\pm auv \leq |a| |uv| \leq \frac{|a|}{2} (u^2 + v^2) \quad (3.23)$$

Using (3.23) and integrating by parts, (3.22) becomes

$$\begin{aligned}\dot{v} \leq & - \int_0^1 \left(\frac{\partial u}{\partial x} \right)^2 \left[a_{11} - \left| \frac{a_{12} (M + 1)}{2} \right| \right] dx \\ & - \int_0^1 \left(\frac{\partial v}{\partial x} \right)^2 \left[2M - \left| \frac{a_{12} (M + 1)}{2} \right| \right] dx \\ & + \int_0^1 u^2 F_u dx + \int_0^1 v^2 F_v dx \quad (3.24)\end{aligned}$$

where

$$F_u = a_{12} M\beta f_y - a_{11} f_y + |2M\beta f_y - a_{11} f_z + a_{12} (M\beta f_z - f_y)| \quad (3.25)$$

$$F_v = 2M\beta f_z - a_{12} f_z + |2M\beta f_y - a_{11} f_z + a_{12} (M\beta f_z - f_y)| \quad (3.26)$$

Since

$$u^2 \leq (1 - x) \int_0^1 \left(\frac{\partial u}{\partial x} \right)^2 dx \quad (3.27)$$

(3.24) can be written as

$$\begin{aligned} \dot{V} &\leq \int_0^1 \left(\frac{\partial u}{\partial x} \right)^2 dx \left[\int_0^1 (1-x) F_u dx - a_{11} - \frac{a_{12}(M+1)}{2} \right] \\ &+ \int_0^1 \left(\frac{\partial v}{\partial x} \right)^2 dx \left[\int_0^1 (1-x) F_v dx - 2M - \frac{a_{12}(M+1)}{2} \right] \end{aligned} \quad (3.28)$$

Thus, for asymptotic stability, the sufficient conditions are

$$\int_0^1 (1-x) F_u dx < a_{11} - \frac{a_{12}}{2} (M+1) \quad (3.29)$$

$$\int_0^1 (1-x) F_v dx < 2M - \frac{a_{12}}{2} (M+1) \quad (3.30)$$

Comparing (3.29) and (3.30) with (2.35) and (2.36), respectively, it is clear that both sets of sufficient conditions are equivalent if the following relations hold

$$p_1 = a_{11}, \quad p_2 = 2, \quad p_3 = a_{12}$$

Notice, these transformations affect F_u and F_v as well. There is, of course, no loss of generality in having set $p_2 = 2$. This merely acts as a sort of scaling factor, in that, although the numbers change on both sides of the inequalities, the same conclusions hold for each steady state. It amounts to multiplying the matrix \underline{P} by a constant. The results are shown in Table 4 which, if a comparison is made, can be found to correspond closely to Table 1.

TABLE 4

N	<u>P</u> ₁	<u>P</u> ₂	<u>MATRIX</u>	STEADY STATE	INEQUALITY (3.29)		INEQUALITY (3.30)		COMMENT
					L.H.S.	R.H.S.	L.H.S.	R.H.S.	
1	2	2	0	1	0.2543	2	0.6988	2	Stable
	2	2	0	2	3.448	2	12.074	2	No conclusion
	2	2	0	3	-51.74	2	34.57	2	No conclusion
	1	2	1.4	3	-0.7649	-0.4	0.1471	0.6	Stable
2	2	2	0	1	0.2600	2	0.4973	1	Stable
	2	2	0	2	3.678	2	8.648	1	No conclusion
	2	2	0	3	-61.15	2	18.66	1	No conclusion
	0.35	2	0.7	3	-3.514	-0.1755	0.4345	0.4744	Stable

3.5 Another Example: The Tubular Reactor Problem

From the discussion on the tubular reactor problem in chapter 2, recall the transformed equations (2.54) and (2.55)

$$\frac{\partial \xi}{\partial t} = \frac{\partial^2 \xi}{\partial s^2} + \xi(\alpha f_y - \frac{N^2}{4}p) + \alpha n f_z \quad (3.31)$$

$$\frac{\partial n}{\partial t} = \frac{\partial^2 n}{\partial s^2} + n(v f_z - \frac{N^2}{4}p) + v \xi f_y \quad (3.32)$$

with the corresponding boundary conditions

$$\xi(t,0) = n(t,0) = 0,$$

$$\frac{\partial \xi}{\partial s}(t,1) = -\frac{N}{2}p \xi(t,1), \quad (3.33)$$

and

$$\frac{\partial n}{\partial s}(t,1) = -\frac{N}{2}p n(t,1)$$

Proceeding exactly as in the first example easily leads to an equation which is identical to (2.63) except that, as in the previous example, the following changes occur

$$p_1 = a_{11}, p_2 = 2 \text{ and } p_3 = a_{22}$$

Thus, it is obvious that the same Liapunov functional will result if the same inequalities are used. The stability results obtained using the above parameters are shown in Table 5.

TABLE 5

STEADY STATE #	P MATRIX			INEQUALITY (2.75)		INEQUALITY (2.76)		COMMENT
	P ₁	P ₂	P ₃	L.H.S.	R.H.S.	L.H.S.	R.H.S.	
1	2	2	0	-148.61	2	-98.232	2	Stable
2	2	2	0	370.12	2	575.88	2	No conclusion
3	2	2	0	2195.1	2	973.34	2	No conclusion
3	.25	2	-.875	-5.04	-1.50	-157.86	.25	Stable

3.6 Conclusions

The method has been applied to two examples in this chapter. In both cases the Liapunov functional generated was the same (within a constant) as the one chosen for use in the generalized quadratic form method. This was not merely by coincidence, but rather, as planned. It was just a question of how to pick the values of a_{ij} . Choosing other values, for example, in either case, let $a_{12} = 0$, results in a different functional. In fact, in the catalyst particle problem with $a_{12} = 0$, the functional which will be obtained will correspond to a constant multiple of the functional chosen by Berger and Lapidus. Also it is quite probable that, by choosing very different values for a_{ij} , more complicated types of Liapunov functionals will result which will prove stability of both the first and third steady states for that corresponding system. The aim of using this method should always be to try to find the simplest form of Liapunov functional which will suffice. In that way, the job of maneuvering the equations into a form from which sufficient conditions arise is very much easier.

When using the variable gradient method for either lumped or distributed systems it is wise to keep the constant and variable parts of the a_{ij} 's as simple as possible. The way in which the values are chosen depends

very much on the experience of the analyst and his knowledge of the particular plant which he is studying.

CHAPTER 4

CONCLUSIONS AND SUGGESTIONS
FOR FUTURE RESEARCH4.1 Conclusions

The author feels that there are two main contributions made by this thesis. Firstly, the use of a non-identity matrix \underline{P} in the Liapunov functional and, secondly, the extension of the variable gradient method to distributed parameter systems.

The use of a non-identity matrix in the Liapunov functional is a direct extension of the quadratic form used frequently as a Liapunov function for determining stability of systems described by ordinary differential equations. It has been shown here that there are advantages to using this general functional form. Whereas the special case ($\underline{P}=\underline{I}$) used by Berger and Lapidus proved stability for steady state 1 in both examples treated, no conclusion about stability was possible for the other two steady states. However, by using a non-identity matrix it was possible to establish stability of steady state 3 as well. It has also been shown that when using a non-identity matrix in the Liapunov functional, retention of all the terms in the inequalities derived is necessary as otherwise inconclusive results are obtained.

The extension of the variable gradient method of generating Liapunov functions to the case of

distributed parameter systems has been described through two examples. This method yielded results very similar to those obtained by the other method used on the same examples. It has been shown that the Liapunov functionals which were arrived at by the variable gradient method are very similar to the ones used in the first method. This is due to the choice of the variable parameters at hand. However, the end results were obtained somewhat more systematically. The variable gradient method should still be classified as a trial and error method although each trial (if more than one is necessary) is carried out in a more straightforward manner.

It should be mentioned that in both of the methods presented here, there is the requirement that the system equations be at least of second order. This is necessary for using a matrix. It has, however, been shown for the adiabatic tubular reactor problem that results can be obtained by first considering the more general problem and then reducing the final inequalities to the adiabatic case. The adiabatic case cannot be treated directly by either method since the original transient equations of the reactor have been reduced to a single equation.

4.2 Suggestions for Future Research

The application of Liapunov stability theory to distributed parameter systems is still in its infancy.

There need to be developed general methods for constructing Liapunov functionals for various classes of systems. Methods which could deal with the nonlinear problem directly without linearization would be more reliable, in that they would probably yield sharper results.

The variable gradient technique, illustrated here by means of two examples, seems promising and should be further developed for use on more complicated types of systems.

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APPENDIX 1

APL PROGRAMS

For the interested reader, the following APL programs are listed for ready reference. It was mainly the use of these functions that yielded the results of this thesis.

```

∇RKG[□]∇
    ∇ R←T RK G X;TT;IT;J;Q1;Q2;Q3;SN;XX;K ;TSTEP
[ 1] →(1 2 3 =ρ,RCON)/ 3 4 5
[ 2] →0,R←10×ρ□←'INITIAL TIME MUST BE SPECIFIED IN RCON'
[ 3] RCON←RCON,1E-6
[ 4] RCON←RCON,1E-5×(T←,T)[ρ,T]-RCON[1]
[ 5] SN←×RCON[3]×IT=IT←RCON[1]×(T=T←,T)[1]
[ 6] J←4,R←1~TMIN=TMIN←0.02×T[ρT]-IT
[ 7] X←(4,ρ,X)ρX
[ 8] TSTEP←SN×└/K←|(T[1]-IT),0.02×T[ρT]-IT
[ 9] TT←IT
[10] Q1←TSTEP×TT SET X[1;]
[11] Q2←TSTEP×(TT+TSTEP÷2) SET X[1;]+Q1÷2
[12] Q3←TSTEP×(TT+TSTEP÷2) SET X[1;]+Q2÷2
[13] X[J;]←X[1;]+0.16666666666667×Q1+(2×Q2+Q3)+TSTEP×(
    TT+TT+TSTEP) SET X[1;]+Q3
[14] →(2 1 =J←J-1)/ 16 17
[15] →9,TSTEP←TSTEP÷2
[16] →10,,X[1 3 ;]←X[3 1 ;]
[17] →((XX←└/|-/[1] X[2 4 ;])≤RCON[2])/22+K[2]>K[1]
[18] X[1 4 ;]←X[3 1 ;]
[19] TMIN←SN×(|TMIN)└|TSTEP
[20] →(32×1(|TSTEP)<|RCON[3]),2 1,TSTEP←TSTEP÷2
[21] →9,J←3
[22] TSTEP←SN×└/K←|(0.5×T[1]-TT),TSTEP←TSTEP+TSTEP×XX<
    RCON[2]÷50
[23] TSTEP←TSTEP×2
[24] IT←TT
[25] J←4
[26] X[1;]←X[2;]
[27] →((|T[1]-TT)>|TSTEP÷2)/10
[28] R←R,TT,X[2;]
[29] TSTEP←SN×K[1]←└/K[2],|IT-T←1+T
[30] →(0≠ρT)/10-2×TSTEP=0
[31] →0,,R←Q(((ρR)÷1+(ρX)[2]),1+(ρX)[2])ρR
[32] →3 1,ρ□←'STEP SIZE HAS BECOME SMALLER THAN INPUT CON
    TROL--RCON[3]'
```

∇

$\nabla SET[\square] \nabla$

```

     $\nabla R \leftarrow T \text{ } SET \text{ } X; N; B; A; Q$ 
[1]  $R \leftarrow X[2], (30 \times X[2]) + 22500000000000 \times (X[1] -$ 
     $1.4) \times * - 30 \div X[1]$ 
 $\nabla$ 

```

$\nabla FEFN[\square] \nabla$

```

     $\nabla II \leftarrow Z \text{ } FEFN \text{ } P; DFY; DFZ$ 
[1]  $A \leftarrow 2.25 \times 10 * 13$ 
[2]  $DFY \leftarrow * - 30 \div Z[2;]$ 
[3]  $DFZ \leftarrow DFY \times 30 \times (1.4 - Z[2;]) \div 0.4 \times Z[2;] * 2$ 
[4]  $FE \leftarrow (P[1] \times (A \times DFY) - 225) + (P[3] \times$ 
     $0.4 \times A \times DFY) + SS \leftarrow 0.5 \times |(P[1] \times A \times DFZ) + (P[3] \times$ 
     $0.4 \times A \times DFZ) - 450 - A \times DFY| + P[2] \times 0.4 \times A \times DFY$ 
[5]  $FN \leftarrow (P[2] \times (0.4 \times A \times DFZ) - 225) + (P[3] \times A \times DFZ) + SS$ 
[6]  $II \leftarrow (3, \rho Z[1;]) \rho Z[1;], (Z[1;] \times FE), Z[1;] \times FN$ 
 $\nabla$ 

```

$\nabla INTEGRAL1[\square] \nabla$

```

     $\nabla R \leftarrow INTEGRAL1 \text{ } X; T; O$ 
[1]  $\rightarrow 3 \times 12 = \rho \rho X$ 
[2]  $\rightarrow 0, \rho \square \leftarrow 'REQUIRE MATRIX ARGUMENT'$ 
[3]  $T \leftarrow X[1;]$ 
[4]  $X \leftarrow 1 \ 0 \ + X$ 
[5]  $\rightarrow 8 \times 1 (2 \leq \rho T) \wedge \wedge / T = H \leftarrow 1 + T \leftarrow 1 + T - 1 \phi T$ 
[6]  $R \leftarrow (0 \ 1 \ + X + -1 \phi X) + . \times T \div 2$ 
[7]  $\rightarrow 0$ 
[8]  $R \leftarrow (H \div 6) \times X + . \times 2, ((-1 - O - \rho T) \rho \ 8 \ 4), (1 + O) \rho \ 2 \ 0 \ +$ 
     $3 \times O \leftarrow 2 \mid \rho T$ 
 $\nabla$ 

```


$\nabla TEST[\square] \nabla$

```

     $\nabla Z TEST P;Y$ 
[1]   $II \leftarrow Z FEFN P$ 
[2]   $Y \leftarrow INTEGRAL1 II$ 
[3]   $\rightarrow (CA \leftarrow Y[1] < P[1] - 2 \times |P[3]|) / 5$ 
[4]  'CONDITION A FAILS'
[5]   $\rightarrow (CB \leftarrow Y[2] < P[2] - 2 \times |P[3]|) / 7$ 
[6]  'CONDITION B FAILS'
[7]   $\rightarrow (CA \wedge CB) / 10$ 
[8]  'NO CONCLUSION LHS(A) = ' ; Y[1]; '           LHS(B) = ' ; Y[
   2]
[9]   $\rightarrow 0$ 
[10] 'THIS SOLN. IS STABLE , LHS(A) = ' ; Y[1]; '      LH
     S(B) = ' ; Y[2]
 $\nabla$ 

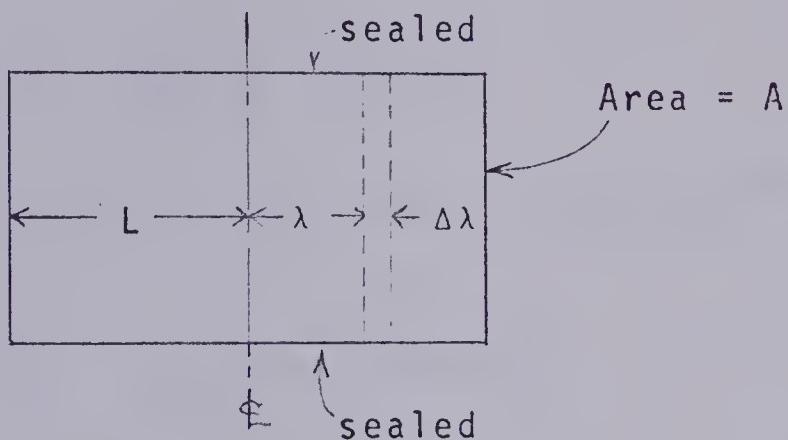
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APPENDIX 2

DERIVATION OF EQUATIONS

a) Catalyst Particle Problem

In order to treat a one-dimensional problem consider the catalyst particle to have the form of a flat slab with sealed edges as shown.



A material balance over this element yields

$$\left[\text{Rate of transport in} \right] - \left[\text{Rate of transport out} \right] - \left[\text{Rate of reaction} \right] = \left[\text{Time rate of change of concentration} \right]$$

$$A \times D \left[\frac{\partial c}{\partial \lambda} \Big|_{\lambda + \Delta \lambda} - \frac{\partial c}{\partial \lambda} \Big|_{\lambda} \right] - A \times \Delta \lambda \times \frac{dn}{d\tau} = \frac{\partial c}{\partial \tau} \times A \times \Delta \lambda \quad (\text{A2.1})$$

Dividing through by $A \times \Delta \lambda$ and taking the limit as $\Delta \lambda \rightarrow 0$ yields

$$D \frac{\partial^2 c}{\partial \lambda^2} - \frac{dn}{d\tau} = \frac{\partial c}{\partial \tau} \quad (\text{A2.2})$$

where D = the effective diffusion coefficient

c = concentration

$\frac{dn}{d\tau}$ = per unit volume reaction rate

If $c = c_0$ at $\lambda = L$, (A2.2) can be written

$$\frac{\partial^2 y}{\partial \lambda^2} - \frac{1}{Dc_0} \frac{dn}{d\tau} = \frac{1}{D} \frac{\partial y}{\partial \tau} \quad (\text{A2.3})$$

where $y = c/c_0$

This may be normalized by letting $x = \lambda/L$.

Then

$$\frac{\partial^2 y}{\partial x^2} - \frac{L^2}{Dc_0} \frac{dn}{d\tau} = \frac{L^2}{D} \frac{\partial y}{\partial \tau} \quad (\text{A2.4})$$

From the work of Weisz and Hicks³⁷ it follows

that

$$\frac{dn}{d\tau} = k_0 c_0 y \exp\left[\frac{\gamma(z-1)}{z}\right] \quad (\text{A2.5})$$

where k_0 = rate constant at the boundary

$$z = T/T_0$$

T = temperature

T_0 = T_0 at the boundary

combining (A2.4) and (A2.5) yields

$$\frac{\partial^2 y}{\partial x^2} - \frac{L^2 k_0}{D} y \exp\left[\frac{\gamma(z-1)}{z}\right] = \frac{L^2}{D} \frac{\partial y}{\partial \tau} \quad (\text{A2.6})$$

or $\frac{\partial^2 y}{\partial x^2} - \phi^2 y \exp\left[\frac{\gamma(z-1)}{z}\right] = \frac{\partial y}{\partial t}$ (A2.7)

where $\phi^2 = \frac{L^2 k_0}{D}$ = Thiele modulus

and $t = \frac{D\tau}{L^2}$

Equation (A2.7) is the same as equation (2.3).

A similar temperature balance on the element yields

$$A \times K \left[\frac{\partial T}{\partial \lambda} \Big|_{\lambda + \Delta \lambda} - \frac{\partial T}{\partial \lambda} \Big|_{\lambda} \right] - A \times \Delta \lambda \times H \times \frac{dn}{d\tau} = \frac{\partial T_p}{\partial \tau} c_p \times A \times \Delta \lambda \quad (\text{A2.8})$$

where K = effective thermal conductivity

H = molar heat of reaction

ρ = density

c_p = heat capacity

In the limit (A2.8) can be written

$$K \frac{\partial^2 T}{\partial \lambda^2} - H \frac{dn}{d\tau} = \rho c_p \frac{\partial T}{\partial \tau} \quad (\text{A2.9})$$

normalizing yields

$$\frac{\partial^2 z}{\partial x^2} - \frac{L^2 H}{K T_0} \frac{dn}{d\tau} = \frac{L^2 \rho c_p}{K} \frac{\partial z}{\partial \tau} \quad (\text{A2.10})$$

$$\text{or } \frac{\partial^2 z}{\partial x^2} - \frac{L^2 H}{K T_0} k_o c_o y \exp \left[\frac{\gamma(z-1)}{z} \right] = \frac{L^2 \rho c_p}{K} \frac{\partial z}{\partial \tau} \quad (\text{A2.11})$$

which can be simplified to

$$\frac{\partial^2 z}{\partial x^2} + \phi^2 \beta y \exp \left[\frac{\gamma(z-1)}{z} \right] = N \frac{\partial z}{\partial t} \quad (\text{A2.12})$$

$$\text{where } \beta = \frac{c_0 H D}{K T_0} = \left(\frac{\Delta T}{T_0} \right)_{\max}$$

$$N = \frac{\rho c_p D}{K} = \text{Lewis number}$$

Equation (A2.12) is the same as (2.4)

b) Adiabatic Tubular Reactor

A similar derivation for equations (2.40) and (2.41) can be found in⁴. For clarity some of the constants are defined here.

$$y = c/c_0$$

$$z = T/T_0$$

where c_0, T_0 occur at the inlet of the reactor.

$$N_p = \frac{v l}{D}$$

where v = fluid velocity within reactor

l = reactor length

$$\alpha = \frac{l^2 K}{D}$$

$$Q = E/RT_0$$

where E = activation energy

and R = gas constant

$$v = \beta \alpha$$

$$\text{where } \beta = \frac{-Hc_0}{T_0 \rho c_p}$$

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